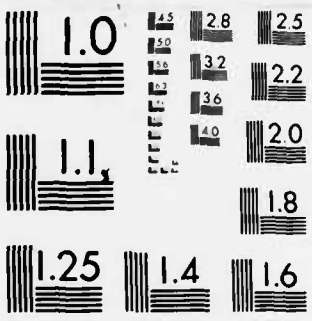
AD-A139 070 JOURNAL OF ENGINEERING THERMOPHYSICS (SELECTED ARTICLES)(U) FOREIGN TECHNOLOGY DIV WRIGHT-PATTERSON AFB OH M GE ET AL. 07 FEB 84 FTD-ID(RS)T-1883-83 1/1

UNCLASSIFIED F/G 20/13 NL

END
DATE FILMED
4-84
DTIC



FTD-ID(RS)T-1883-83

# FOREIGN TECHNOLOGY DIVISION

JOURNAL OF ENGINEERING THERMOPHYSICS

(Selected Articles)



Approved for public release;
distribution unlimited.

# EDITED TRANSLATION

FTD-ID(RS)T-1883-83 7 February 1984

MICROFICHE NR: FTD-84-C-000146

JOURNAL OF ENGINEERING THERMOPHYSICS
(Selected Articles)

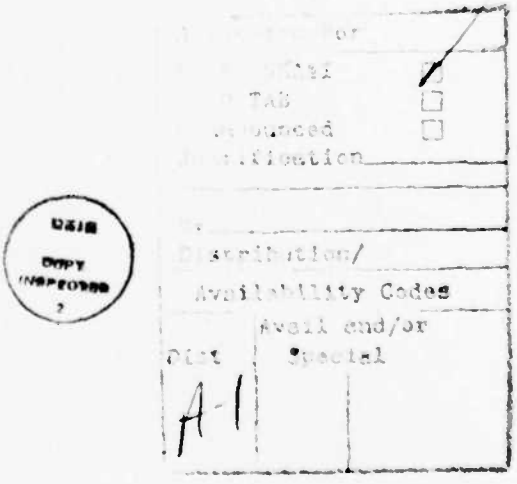
English pages: 19

Source: Gongcheng Rewuli Xuebao, Vol. 3,
Nr. 4, 1982, pp. 323-329; 330-333

Country of origin: China
Translated by: SCITRAN
F33657-81-D-0263
Requester: FTD/SDBS
Approved for public release; distribution unlimited.

Table of Contents





GRAPHICS DISCLAIMER

All figures, graphics, tables, equations, etc. merged into this translation were extracted from the best qulaity copy available.

# Thermodynamic Extrapolation of Rocket Engine Performance Parameters

Ge Minglong

Abstract

In this paper, an isentropic reference line and two partial derivatives with fixed enthalpy were used to establish the extrapolation formulas for rocket engine performance parameters. When the initial enthalpy value of the propellant, combustion chamber pressure, and nozzle exit pressure began to vary, these formulas could be used to carry out extrapolating calculations for specific thrust, characteristic velocity, nozzle area ratio, combustion chamber thermodynamic parameters, and nozzle exit thermodynamic parameters. The formulas in this paper are simple and easy to use. The accuracy is high.

## I. Introduction

The thermodynamic calculation of the theoretical performance characteristics of a rocket engine is a classical case. It has been introduced in Reference 1 as well as in other books and journals concerning rocket engines. This complicated calculation is very useful in the design of a rocket engine. However, it consumes a considerable amount of computer time. Furthermore, it is also inconvenient to organize the great deat of data into volumes. Therefore, the extrapolating calculation problem of the theoretical performance characteristics of a rocket engine had been brought out. Some people gave the formulas in thermodynamic extrapolating calculation.[2-5]

In recent years, along with the availability of pocket electronic calculators, it is even more convenient to use an extrapolation method to calculate the theoretical characteristics of a rocket engine. For this reason, on the basis of presently available extrapolation formulas, more accurate extrapolation formulas were derived in this paper.

## II. Isentropic Reference Line

For a certain propellant composition at a fixed mixture ratio O/F, because its elemental composition is fixed, therefore,

the ideal thermodynamic process of the engine - the isentropic limiting equilibrated expansion process - can be expressed as various isentropic lines such as $c_o t_o e_o e"$, cte,...etc., on the same isentropic diagram as shown in Figure 1 regardless of the same isentropic value ($H_{co}$ or $H_c$) of the propellant as affected by factors such as the environmental temperature. It is also irrespective to the combustion chamber pressure ($P_{co}$, $P_c'$, or $P_c$), and the nozzle exit pressure ($P_{co}$, $P_e'$, $P_e"$ or $P_e$).

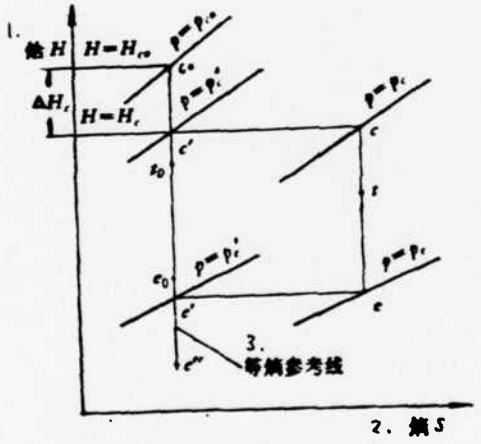



Figure 1. Schematic Diagram of Enthalpy and Entropy

1. enthalpy H
2. entropy S
3. isentropic reference line

For a given propellant initial enthalpy value ($H_{co}$) and combustion chamber pressure ($P_{co}$), it is possible to determine the thermodynamic parameters for a combustion chamber condition point $c_o$ and throat condition point $t_o$ through an accurate thermodynamic calculation. Then, several nozzle exit pressure levels were chosen to calculate the thermodynamic parameters of these nozzle exit condition points ($e_o$, e",...).

Received in December 1981

1. (气氢气氧燃烧剂，混合比 $O/F = 7.9365$，初始焓值 $H_{t_0} = 0$ 大卡/公斤)

| 参数 2. | 燃烧室 3 | 喷嘴 4 | 5. 喷管出口 | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $p_t/p$ | 1 | 1.727 | 10 | 40.827 | 68.046 | 100 | 300 | 400 | 600 | 800 | 1000 | 3000 | 10000 | |
| 6. $\rho$, 公斤/厘米³(绝对) | 68.05 | 39.40 | 6.805 | 1.667 | 1 | 0.6805 | 0.2268 | 0.1701 | 0.1134 | 0.0851 | 0.0680 | 0.0227 | 0.0068 | |
| $T$, K | 3600 | 5506 | 3015 | 2674 | 2556 | 2469 | 2218 | 2151 | 2055 | 1985 | 1930 | 1650 | 1445 | |
| 7. $H$, 大卡/公斤 | 0 | −245.9 | −942.0 | −1412.1 | −1566.2 | −1676.9 | −1968.2 | −2038.7 | −2133.9 | −2198.6 | −2247.1 | −2464.9 | −2661.7 | |
| 8 $M$, 公斤/公斤克尔 | 15.752 | 15.974 | 16.656 | 17.148 | 17.510 | 17.423 | 17.702 | 17.761 | 17.634 | 17.878 | 17.907 | 17.992 | 18.014 | |
| 9. $c_p$, 大卡/公斤 K | 2.5901 | 2.5481 | 2.2704 | 1.9066 | 1.7508 | 1.6279 | 1.2694 | 1.1787 | 1.0577 | 0.9784 | 0.9217 | 0.7137 | 0.6126 | |
| $\left(\frac{\partial \ln M}{\partial \ln \rho}\right)_T$ | 0.05008 | 0.04509 | 0.02958 | 0.01844 | 0.01484 | 0.01234 | 0.00633 | 0.00508 | 0.00358 | 0.00270 | 0.00212 | 0.00046 | 0.00004 | |
| $\left(\frac{\partial \ln M}{\partial \ln T}\right)_\rho$ | −0.0458 | −0.0001 | −0.6118 | −0.4308 | −0.3610 | −0.3125 | −0.1786 | −0.1479 | −0.1090 | −0.0849 | −0.0686 | −0.0171 | −0.0018 | |
| $D_T = \left(\frac{\partial \ln T}{\partial \ln \rho}\right)_s$ | 0.04120 | 0.01906 | 0.03215 | 0.02619 | 0.02380 | 0.02190 | 0.01579 | 0.01404 | 0.01148 | 0.00965 | 0.00826 | 0.00267 | 0.00032 | |
| $D_M = \left(\frac{\partial \ln M}{\partial \ln \rho}\right)_s$ | 0.01521 | 0.01564 | 0.00991 | 0.00716 | 0.00620 | 0.00550 | 0.00351 | 0.00300 | 0.00253 | 0.00188 | 0.00155 | 0.00041 | 0.00004 | |
| $D_T = \left(\frac{\Delta T}{\Delta \ln \rho}\right)_s$ | 357° | 516.4 | 279.6 | 242.4 | 230.9 | 226.0 | 220.4 | 232.9 | 236.8 | 243.8 | 245.2 | 255.2 | 255.0 | |
| $D_M = \left(\frac{\Delta M}{\Delta \ln \rho}\right)_s$ | −0.424° | −0.486 | −0.3804 | −0.3498 | −0.5170 | −0.2936 | −0.2519 | −0.2051 | −0.1800 | −0.1513 | −0.1293 | −0.0775 | −0.0183 | |
| $D_H = \left(\frac{\Delta H}{\Delta \ln \rho}\right)_s$ | 904° | 450.8 | 346.4 | 334.2 | 301.5 | 287.6 | 265.1 | 245.1 | 214.8 | 225.4 | 216.2 | 198.5 | 164.9 | |
| $D_{DT} = \left(\frac{\Delta D_T}{\Delta \ln \rho}\right)_s$ | 0.00380° | 0.0039160 | 0.0039390 | 0.0042370 | 0.0046770 | 0.0049360 | 0.0055610 | 0.0060810 | 0.0063140 | 0.0067470 | 0.0070970 | 0.0050950 | 0.001450 | |
| $D_{DM} = \left(\frac{\Delta D_M}{\Delta \ln \rho}\right)_s$ | 0.00389° | 0.0039440 | 0.0022980 | 0.0019550 | 0.0018780 | 0.0018190 | 0.0018110 | 0.0017710 | 0.0016520 | 0.0015470 | 0.0014710 | 0.0010190 | 0.000407 | |

14 • 外插得到的数据

Table 1. Parameters on the Isentropic Reference Line

1. (hydrogen gas and oxygen gas propellant, mixing ratio O/F=7.9365, initial enthalpy value $H_{co}$=0 Kcal/kg)
2. parameter
3. combustion chamber
4. throat
5. nozzle exit
6. P, kg/cm$^3$ (absolute)
7. H, Kcal/kg
8. M, kg/kg mole
9. Cp Kcal/kg K
10. *data obtained through extrapolation.

/325

On the isentropic line $c_o t_o e_o e''$, there are several points with known values of sych parameters as pressure ratio $p_c/p$, pressure p, temperature T, enthalpy H, molecular weight M, and constant pressure specific heat cp, as well as partial derivatives such as $\left(\frac{\partial \ln M}{\partial \ln p}\right)_T$ and $\left(\frac{\partial \ln M}{\partial \ln T}\right)_p$ (the calculation formulas and methods of two partial derivatives have been shown in References 1 and 4). Therefore, this isentropic line can be used as a reference line in the extrapolation. The parameters of a typical isentropic reference line are listed in Table 1. The parameters in the upper half of the table came from Reference 5.

On an isentropic line, the thermodynamic parameters of a point other than a parametric point can be calculated by using the following extrapolation formula in approximation:

$$\left.\begin{aligned} F &= Q \ln \rho \\ (\Delta F)_i &= Q (\Delta \ln \rho)_i \end{aligned}\right\} \qquad (1)$$

where F repreents parameters such as T, H, M...etc. Q is the extrapolation coefficient, which is determination by the parameters of the two known neighboring points.

With respect to the isentropic reference line in Table 1, the results of the calculation of the extrapolation coefficients such as $Q_T$, $Q_M$, and $Q_H$ are listed in the lower half of the table.

## III. Isenthalpic Partial Derivatives and Isenthalpic Correlations

Referring to the relevant formulas in References 4 and 5, the two isenthalpic partial derivatives used in this paper can be expressed by using the following formulas:

$$D_T = \left(\frac{\partial \ln T}{\partial \ln p}\right)_H = \frac{-R}{c_p M}\left(\frac{\partial \ln M}{\partial \ln T}\right)_p \tag{2}$$

$$D_M = \left(\frac{\partial \ln M}{\partial \ln p}\right)_H = \frac{-R}{c_p M}\left(\frac{\partial \ln M}{\partial \ln T}\right)_p^2 + \left(\frac{\partial \ln M}{\partial \ln p}\right)_T \tag{3}$$

where R is the commonly used gas constant (1.98726 Kcal/kg mole K).

With respect to the isentropic reference line in Table 1, the values of $D_T$, $D_M$, $Q_{DT}$ and $Q_{DM}$ calculated from the formulas given above are listed in the lower half of the table.

The correlations of temperature and molecular weight on an isentropic line are

$$(\Delta \ln T)_H = D_T(\Delta \ln p)_H \tag{4}$$

$$(\Delta \ln M)_H = D_M(\Delta \ln p)_H \tag{5}$$

Substituting the expression of the first law of thermodynamics and the equation of state into the differential equation of entropy, one gets

$$ds = \frac{dH}{T} - \frac{R}{M}\frac{dp}{p} \tag{A}$$

For an isenthalpic line (dH=0), the formula gives

$$(\Delta s)_H = -\frac{R}{M}(\Delta \ln p)_H \tag{6}$$

## IV. Establishment of Extrapolation Formulas

### 1. Combustion Chamber Thermodynamic Parameters and Formula for Characteristic Velocity.

When the initial enthalpy of the propellant $H_C \neq H_{CO}$ and the combustion chamber pressure $p_C \neq p_{CO}$, based on $\Delta H_C = H_C - H_{CO}$ and the known data at point $c_o$, it is possible to calculate the parameters of point c' in Figure 1 using equation (1). Then, according to the parameters at point c' and $p=P_C$, the parameters at point c can be calculated according to equations (4) and (5). Finally, the combustion chamber temperature and moelcular formulas can be obtained:

$$T_c = \left(T_{co} + \frac{Q_T \Delta H_c}{Q_H}\right) \exp\left[\left(D_{TCO} + \frac{Q_{DT}\Delta H_c}{Q_H}\right)\left(\ln \frac{p_c}{p_{co}} - \frac{\Delta H_c}{Q_H}\right)\right] \tag{7}$$

/326

$$M_c = \left(M_{co} + \frac{Q_M \Delta H_c}{Q_H}\right) \exp\left[\left(D_{MCO} + \frac{Q_{DM}\Delta H_c}{Q_H}\right)\left(\ln \frac{p_c}{p_{co}} - \frac{\Delta H_c}{Q_H}\right)\right] \tag{8}$$

Since the characteristic velocity c* is proprotional to $\sqrt{T_C/M_C}$, the extrapolation formula for characteristic velocity can be written as

$$c^* = c_o^* \sqrt{T_c M_{co}/M_c T_{co}} \tag{9}$$

### 2. Formulas of Thermodynamic Parameters at the Nozzle Exit ($p=P_C$)

Applying equation (6) between points c and c', and e and e'

$$\ln \frac{p_{c'}}{p_c} = \frac{M_{c'}}{M_{c'}} \ln \frac{p_{c'}}{p_c} \tag{A}$$

Substitute equation (1) into this formula, one gets

$$\ln \frac{p_{c'}}{p_{co}} = \ln \frac{p_c}{p_{co}} + \frac{M_{co}\left(\frac{\Delta H_c}{Q_H} - \ln \frac{p_c}{p_{co}}\right)}{M_{co} + \frac{Q_M \Delta H_c}{Q_H}} \tag{10}$$

where $M_{eo}$ is the approximate value of $M_e'$. It is the known molecular weight of $p = p_{eo}$ on the isentropic reference line close to $p_e'$. In order to select $p_{eo}$ so that $M_{eo}$ can be determined, the initial value of $p_e'$ can be calculated according to the following formula:

$$p_{e'} = p_c \exp\left[\frac{M_{e''}}{M_{co}}\left(\frac{\Delta H_c}{Q_H} - \ln \frac{p_c}{p_{co}}\right)\right] \tag{11}$$

This formula was obtained as an approximation of equation (10). The $M_e''$ in the equation is the known molecular weight of the lowest point on the isentropic reference point.

The values near $p_{eo}$ were adopted as the extrapolation coefficients $Q_T$, $Q_{DT}$, $Q_M$, $Q_{DM}$, $Q_H$, in equations (7), (8), (10) and (11). When $\Delta H_c < 0$, the average value of $c_o - t_o$ was used. When $\Delta H_c > 0$, the values for $p > p_{co}$ were used.

Based on the known data at point $e_o$ and the value of $\ln \frac{P_e}{P_{eo}}$ calculated from equation (10), the parameters at point e' can be calculated using equation (1). Then, based on the parameters at point e' and $P = P_c$, the parameters at point e can be calculated from equations (4) and (5). Thus, the formulas for nozzle exit temperature and molecular weight were obtained.

$$T_e = \left(T_{eo} + Q_T \ln \frac{p_{e'}}{p_{eo}}\right) \exp\left[\left(D_{Teo} + Q_{DT} \ln \frac{p_{e'}}{p_{eo}}\right)\left(\ln \frac{p_e}{p_{eo}} - \ln \frac{p_{e'}}{p_{eo}}\right)\right] \tag{12}$$

$$M_e = \left(M_{eo} + Q_M \ln \frac{p_{e'}}{p_{eo}}\right) \exp\left[\left(D_{Meo} + Q_{DM} \ln \frac{p_{e'}}{p_{eo}}\right)\left(\ln \frac{p_e}{p_{eo}} - \ln \frac{p_{e'}}{p_{eo}}\right)\right] \tag{13}$$

3. Formulas for parameters such as the specific Thrust

Substituting $H_c = H_{c'} \simeq H_{co} + \Delta H_c$ and $H_e = H_{e'} = H_{eo} + Q_H \ln \frac{P_{e'}}{P_{eo}}$ into the specific thrust formula at the designed altitude $I = 294.98 \sqrt{(H_c - H_e)/1000}$, we get

$$I = 9.328 \sqrt{H_{eo} + \Delta H_c - H_{eo} - Q_H \ln \frac{p_{e'}}{p_{eo}}} \tag{14}$$

The extrapolating coefficients $Q_T$, $Q_{DT}$, $Q_M$, $Q_{DM}$, and $Q_H$ in equations (12) through (14) adopted their values at near $P_{eo}$. When $\ln \frac{P_{e'}}{P_{eo}} < 0$, the values less than those of $P_{eo}$ were used. When $\ln \frac{P_{e'}}{P_{eo}} > 0$, the values greater than those of $P_{eo}$ were used.

The nozzle exit area ratio and the nozzle area ratio are calculated from the following formulas: /327

$$f_e = 86.50 T_e / I p_e M_e \tag{15}$$

$$\varepsilon = f_e g p_c / c^* \tag{16}$$

## V. Accuracy of Extrapolation Formulas

On the basis of the formulas given above, it is possible to carry out extrapolation calculations. For a hydrogen oxygen propellant with a mixing ratio O/F=7.9365, some of the results of extrapolation, such as nozzle area ratio, characteristic velocity, combustion chamber temperature, and specific thrust at designed altitude, are listed in Tables 2, 3, 4 and Figure 2, respectively. For comparison, the results[5,6] of the corresponding accurate calculation and the extrapolated calculation in Reference 5 are also listed in these figures and tables.

| $p_c/p$ | 1. 液氧液氢，焓值 $H_c = -190.6$ 大卡/公斤 | | | 2. 气氢臭氧，焓值 $H_c = 629.1$ 大卡/公斤 | | |
|---|---|---|---|---|---|---|
| | 3. 精确值 | 4. 本文的外推值 | 5. 文献5的外推值 | 6. 精确值 | 7. 本文的外推值 | 8. 文献5的外推值 |
| 10 | 2.468 | 2.476 | 2.289 | 2.466 | 2.459 | 2.337 |
| 40.83 | 7.151 | 7.188 | 7.130 | 7.169 | 7.196 | 7.279 |
| 68.05 | 10.75 | 10.80 | 10.77 | 10.81 | 10.77 | 11.00 |
| 100 | 14.69 | 14.74 | 14.70 | 14.81 | 14.70 | 15.01 |
| 300 | 36.28 | 36.40 | 35.70 | 37.02 | 37.05 | 36.45 |
| 400 | 46.04 | 46.19 | 45.04 | 47.22 | 47.29 | 45.98 |
| 600 | 64.44 | 64.58 | 62.49 | 66.66 | 66.55 | 63.80 |
| 800 | 81.77 | 81.90 | 78.83 | 85.21 | 84.97 | 80.49 |
| 1000 | 98.31 | 98.41 | 94.40 | 103.2 | 103.6 | 96.38 |

Table 2. Comparison of the Nozzle Area Ratio Calculated by Extrapolation with Its Accurate Value

(hydrogen oxygen propellant, mixing ratio O/F=7.9365, combustion chamber pressure $p_c$=6.805Kg/cm$^2$, absolute)

1. liquid hydrogen, liquid oxygen, enthalpy $H_c$ = -190.6 Kcal/kg
2. gas hydrogen, ozone, enthalpy $H_c$ = 629.1 Kcal/kg
3. accurate value
4. extrapolated value in this work
5. extrapolated value in Reference 5
6. accurate value
7. extrapolated value in this work
8. extrapolated value in Reference 5.

| 1. 燃烧室压力 $p_c$ 公斤/厘米², 绝对 | 气氢气氧,焓值 $H_c=0$ 2. 大卡/公斤 | | | 液氢液氧,焓值 $H_c=$ 3. −190.6 大卡/公斤 | | | 气氢臭氧,焓值 $H_c=629.1$ 4. 大卡/公斤 | | |
|---|---|---|---|---|---|---|---|---|---|
| | 5. 精确值 | 6. 外推值 | | 9. 精确值 | 10. 外推值 | | 13 精确值 | 14 外推值 | |
| | | 7. 本文 | 8. 文献 5 | | 11. 本文 | 12. 文献 5 | | 15. 本文 | 16. 文献 5 |
| 68.05 | 2197 | 2197 | 2197 | 2156 | 2156 | 2157 | 2324 | 2326 | 2329 |
| 40.83 | 2184 | 2182 | 2184 | 2144 | 2142 | 2144 | 2308 | 2310 | 2316 |
| 6.805 | 2136 | 2132 | 2139 | 2099 | 2094 | 2099 | 2251 | 2254 | 2271 |

17. 注: 表中特征速度数值的单位是米/秒

Table 3. Comparison of the Extrapolated Characteristic Velocity with Its Accurate Value (hydrogen-oxygen propellant, mixing ratio O/F = 7.9365)

1. combustion chamber pressure $p_c$, $Kg/cm^2$, absolute
2. gas hydrogen, gas oxygen, enthalpy $H_c = 0$ Kcal/kg)
3. liquid hydrogen, liquid oxygen, enthalpy $H_c = -190.6$ Kcal/kg
4. gas hydrogen, ozone, enthalpy $H_c = 629.1$ Kcal/kg
5. accurate value
6. extrapolated value
7. this work
8. Reference 5
9. accurate value
10. extrapolated value
11. this work
12. Reference 5
13. accurate value
14. extrapolated value
15. this work
16. Reference 5
17. Note: the unit for the numerical value of characteristic velocity in the table is m/sec.

| 1. 燃烧室压力 $p_c$,公斤/厘米$^2$,绝对 | 1.02 | 2.04 | 4.08 | 10.21 | 20.42 | 40.83 | 61.25 | 81.56 |
|---|---|---|---|---|---|---|---|---|
| 2. 精确值 | 3039 | 3127 | 3217 | 3341 | 3437 | 3534 | 3591 | 3632 |
| 3. 本文的外推值 | 3053 | 3138 | 3225 | 3344 | 3437 | 3533 | 3590 | 3631 |

4. 注: 表中燃烧室温度数值的单位是K

Table 4. Comparison of Extrapolated Combustion Chamber Temperature with Its Accurate Value

(liquid hydrogen - liquid oxygen propellant, mixing ratio O/F = 7.9365)

1. combustion chamber pressure, $p_c$ Kg/cm$^2$ absolute
2. accurate value
3. extrapolated value in this work
4. Note: the unit of combustion chamber pressure in the table is K.

From Tables 2 through 4 and Figure 2 one can see that the /328 accuracy of the extrapolation formulas in this paper is relatively high. They are suited for the extrapolation of the actual parameters of a rocket engine.

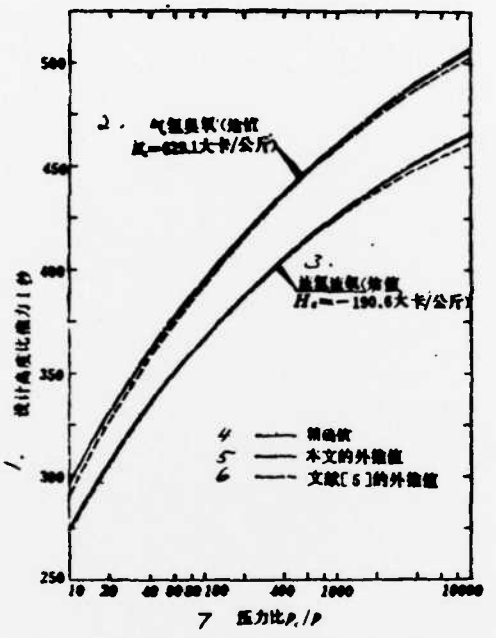



Figure 2. Comparison of Extrapolated Specific Thrust at Designed Altitude and Its Accurate Value

(hydrogen-oxygen propellant, mixing ratio O/F=7.9365, combustion chamber pressure $p_c$ = 6.805 Kg/cm$^2$, absolute)

1. specific thrust at designed altitude, I, sec.
2. gas hydrogen-ozone (enthalpy $H_c$ = 629.1 Kcal/kg)
3. liquid hydrogen-liquid oxygen (enthalpy $H_c$ = -190.6 Kcal/kg)
4. accurate value
5. extrapolated value in this work
6. extrapolated value in Reference (5)
7. pressure ratio $P_c/P$

REFERENCES

[1] S. Gordon, F.J. Zeleznik, and V.N. Huff: A general method for automatic computations of equilibrium compositions and theoretical rocket performance of propellants, NASA TN D-132, (October 1959).

[2] S. Gordon, and V.N. Huff: Theoretical performance of liquid hydrazine and liquid fluorine as a rocket propellant, NACA RM E53E12, (1953).

[3] L.J. Gordon: Uncertainty in a calculated specific impulse due to an uncertainty in the heat of formation of the propellant, ARS J. 30, (1960), 115-116.

[4] M. Barrere, et al: Rocket Propulsion (Chapter 3), Elsevier Publishing Company, Amsterdam, London, New York, Princeton. 1960.

[5] S. Gordon, and F.J. Zeleznik: Thermodynamic extrapolation of rocket performance parameters, ARS J. 32, (1962), 1195-1202.

[6] G.K. Sievers, et al: Theoretical performance of hydrogen-oxygen rocket thrust chambers, NASA TR R-111, (1961).

# A Thermodynamic Calculation Method Of The Symbolic Formula For A Rocket Engine

/330

Fang Zhaokui

In the past, a chemical formula thermodynamic calculation was widely used in our country. Its special feature is that: the chemical reaction must be correlated to the specific chemical elements of the propellant. This makes it difficult to design a generalized program. The symbolic thermodynamic calculation presented in this paper eliminated the aforementioned difficulty.

## I. Symbolic Elements and Molecular Formula

For a given pair of positive integers i and j, any propellant with j elements and producing i combustion products is defined by a series of symbolic elements $A_j$ and the corresponding symbolic element atomic number $a_j$. The sequential arrangement of the symbolic elements $A_j$:

$$\prod^{j} A_j a_{ji} = A_1 a_{1i} A_2 a_{2i} \cdots A_j a_{ji} \quad (i = 1, 2, \cdots i) \tag{1}$$

would represent the moelcular formula of the $i^{th}$ combustion product after the propellant is combusted. The symbol $\prod^{j}$ denotes the sequential arrangement as shown in equation (1).

For example, in the case of a propellant with four elements C, H, O, and N, the symbolic elements $A_1$, $A_2$, $A_3$, and $A_4$ are used to represent these four elements. Let the $i^{th}$ combustion product be CO. Obviously, according to the definition its symbolic elemental molecular formula is:

$$CO = \prod^{j} A_j a_{ji} = A_1 1 A_2 0 A_3 1 A_4 0 \tag{2}$$

The sequence of i and j and its correlation to the products and elements is arbitrary. However, once the correlation is estabsihed, equation (2) uniquely defines CO.

## II. Chemical Equilibrium Equation of Symbolic Element Combustion Product

Definition: For any molecular combustion product $\prod_j^j A_j a_{ji}$, the dissociation reaction correlated to the symbolic element $A_j$

$$\prod^{i} A_j a_{ji} \longrightarrow \sum^{i} a_{ji} A_j \quad (i = 1, 2 \cdots i) \tag{3}$$

is made to be the chemical equilibrium reaction. Due to the fact that symbolic elements are given a part of the definition of a number, therefore, they obey the conventional multiplication law:

$$a_{ji} \times A_j = \begin{cases} 0 & \text{if } a_{ji}=0 \\ a_{ji}A_j & \text{if } a_{ji}\neq 0 \end{cases} \tag{4}$$

From the chemical equilibrium reaction theory, the chemical equilibrium equation corresponding to (3) is:

$$P_{\prod^{i} A_j a_{ji}} \Big/ \left( P_{A_1}^{a_{1i}} \times P_{A_2}^{a_{2i}} \times \cdots \times P_{A_j}^{a_{ji}} \right) = f_i(T) \quad (i = 1,2 \cdots i) \tag{5}$$

where $P_{\prod^{j} A_j a_{ji}}$ and $P_{A_j}$ represent the partial pressure of the symbolic element molecular product $\prod^{j} A_j a_{ji}$ and atomic product $A_j$ in the combustion process, respectively. $f_i(T)$ is the equilibrium

---

This paper was presented in the Engineering Thermodynamics and Energy Conservation Meeting in Xiamen in August, 1981.

constant of the dissociation reaction at temperature T. If a /331 certain element does not exist in this molecule at all (for example, CO molecule do not contain hydrogen at all), $P_{A_j}^{\circ}=1$ due to the conventional mathematical law. Furthermore, equation (5) is satisfied. Taking the logarithm of equation (5) on both sides, we get:

$$\ln P_{\prod^{i} A_j a_{ji}} = \ln f_i(T) + \sum^{i} a_{ji} \ln P_{A_j} \tag{6}$$

Using equation (6), it is possible to convert the moelcular partial pressure into atomic partial pressure to eliminate the molecular variables. Consequently, the number of equations is greatly reduced.

III. Symbolic Element Propellant Matrix and Its Normalization Treatment

Definition: Assuming that there is a complicated propellant comprised of n types of pure chemical substances, the molecular formula, enthalpy, and weight percent of the mixture of each pure chemical substance are $\prod_{j} A_j a_{jn}$, $H_n$, and $X_n$ (n=1,2.. n), respectively. Then, the characteristics of this propellant can be determined by the matrix

$$A(n, j+2) = \begin{pmatrix} a_{11} & a_{21} & \cdots & a_{j1} & H_1 & x_1 \\ a_{12} & a_{22} & \cdots & a_{j2} & H_2 & x_2 \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ a_{1n} & a_{2n} & \cdots & a_{jn} & H_n & x_n \end{pmatrix} \tag{7}$$

(7) is called the propellant matrix. In the performance calculation, it is only necessary to consider the theoretical characteristics possessed by a unit mass. For this reason:

Definition: Choose the unit mole propellant symbol elemental molecular formula whose molecular weight is 1 as the standardized equivalent formula of the propellant. The process of converting from the initial propellant into the symbolic element propellant equivalent formula is called the normalization process of the symbolic element propellant.

Theory: Assuming that there is a complex propellant (7), $u_j$ is the atomic weight of the symbolic element $A_j$.

The matrix

$$B(n) = \begin{pmatrix} x_1 \Big/ \sum^{j} \mu_j a_{j1} \\ x_2 \Big/ \sum^{j} \mu_j a_{j2} \\ \vdots \\ x_n \Big/ \sum^{j} \mu_j a_{jn} \end{pmatrix} \tag{8}$$

Then, the normalization of the propellant (7) is the realization of the following matrix operation.

$$A(j+1) = A'(n, j+1) \times B(n) = \begin{pmatrix} a_{10} \\ a_{20} \\ \vdots \\ a_{j0} \\ H_0 \end{pmatrix} \tag{9}$$

where A'(n,j+1) is the transformation matrix of the matrix A (n,j+1) which was obtained by eliminating the last column in matrix (7). (9) is a column matrix after normalization. The subscript "0" of a column matrix $a_{j0}$ indicates that it does not belong to the "i" series of the combustion chamber. From equation (9), one can derive

$$\sum^{j} \mu_j a_{j0} = 1 \tag{10}$$

This is a natural result of the normalization treatment. For a dual component propellant, if the incendiary agents corresponding to the forms of (7) and (8) are A(n,j+2) and B(n), the oxidants are A(m,j+2) and B(m), and the mixing ratio is K, then

the normalization process of this complex dual component propellant is: /332

$$A(j+1) = [A'(s, j+1) \times B(s) + KA'(m, j+1) \times B(m)]/(1+K) \qquad (11)$$

The final matrix obtained is a column matrix. The proof for (9), (10), and (11) is omitted.

IV. Basic Equation And Program Design In Symbolic Formula Thermodynamic Calculation

Let us assume a propellant is defined by positive integers i and j and the normalization matrix A(j+1). Then, the standard form of the combustion reaction is:

$$M \prod^{j} A_j a_{ji} \longrightarrow \sum^{i} P_i \prod^{j} A_j a_{ji} \qquad (12)$$

The formula above shows that M moles of propellant produces combustion products $\prod^{j} A_j a_{ji}$ at partial pressure $P_i$ when it combusts. However, when a condensed phase exists, $P_i$ should be considered as the mole number of the condensed phase product. Now, the four sets of basic equations in symbolic formula thermodynamic calculation are re-written as the following:

1. Mass Conservation Equation:

$$a_j = \sum^{i} a_{ji} P_i / M \quad j = 1, 2, \cdots j \qquad (13)$$

2. Energy Conservation Equation:

$$\left.\begin{aligned} H_0 &= \sum^{i} (H_T^0)_i P_i / M \text{ (isenthalpic-combustion chamber state)} \\ S_0 &= \sum^{i} [(S_T^0)_i - \beta_i] P_i / M \text{ (isentropic-combustion chamber state)} \end{aligned}\right\} \qquad (14)$$

3. Chemical Equilibrium Equation:

$$(F_T^0)_i/(RT) + \ln\omega_i - \sum^{j} a_{in}[(F_T^0)_i/(RT) + \ln\omega_i] = 0 \quad i = 1, 2, \cdots i, \tag{15}$$

where $(H_T^0)_i$, $(S_T^0)_i$, and $(F_T^0)_i$ in equations (14) and (15) are the enthalpy, entropy, and free energy of the $i^{th}$ product at temperature T, respectively.

$$\beta_i = \begin{matrix} R\ nP_i & \text{(for gas phase)} \\ 0 & \text{(for condensed phase)} \end{matrix} \qquad w_i = \begin{matrix} P_i & \text{(for gas phase)} \\ 1 & \text{(for condensed phase)} \end{matrix}$$

R is the gas constant of a mole of generalized gas. The formula for the condensed phase is omitted.

4. Dalton's Law

$$P_0 = \sum^{i} P_i \quad \text{(for gas phase only)} \tag{16}$$

Solving the aforementioned equation with known A(n,j+2), A(m,j+2), K, $P_0$, $H_0$, and $\mu_j$ becomes the basic problem in thermodynamic calculation.

In designing the program, it is necessary to linearize the equations. Furthermore, (6) is used to reduce the number of equations. Partial derivative approximation and convergence factor are used to resolve the arbitrariness of the initial value in a large range. We used the BCY language to compile the generalized program for thermodynamic calculation. Several dozens of propellants were calculated on a 109-B computer with success. Due to the limitation of pages, it is not described in detail.

REFERENCES

[1] B.E. Attemacob: ((Principle of Rocket Engine)), National Defense Industry Publishing Co. (1965).

[2] B.J. McBride, S. Heimel, J.G. Ehlers, S. Gordon: "Thermodynamic Properties To 6000 K for Substances Involving the First 18 Elements", NASA SP-3001, (1963).

DISTRIBUTION LIST

DISTRIBUTION DIRECT TO RECIPIENT

| ORGANIZATION | MICROFICHE |
|---|---|
| A205 DMAHTC | 1 |
| A210 DMAAC | 1 |
| B344 DIA/RTS-2C | 9 |
| C043 USAMIIA | 1 |
| C500 TRADOC | 1 |
| C509 BALLISTIC RES LAB | 1 |
| C510 R&T LABS/AVRADCOM | 1 |
| C513 ARRADCOM | 1 |
| C535 AVRADCOM/TSARCOM | 1 |
| C539 TRASANA | 1 |
| C591 FSTC | 4 |
| C619 MIA REDSTONE | 1 |
| D008 NISC | 1 |
| E053 HQ USAF/INET | 1 |
| E403 AFSC/INA | 1 |
| E404 AEDC/DOF | 1 |
| E408 AFWL | 1 |
| E410 AD/IND | 1 |
| E429 SD/IND | 1 |
| P005 DOE/ISA/DDI | 1 |
| P050 CIA/OCR/ADD/SD | 2 |
| AFIT/LDE | 1 |
| FTD | |
| CCN | 1 |
| NIA/PHS | 1 |
| NIIS | 2 |
| LLNL/Code L-389 | 1 |
| NASA/NST-44 | 1 |
| NSA/1213/TDL | 2 |


DATE
ILME